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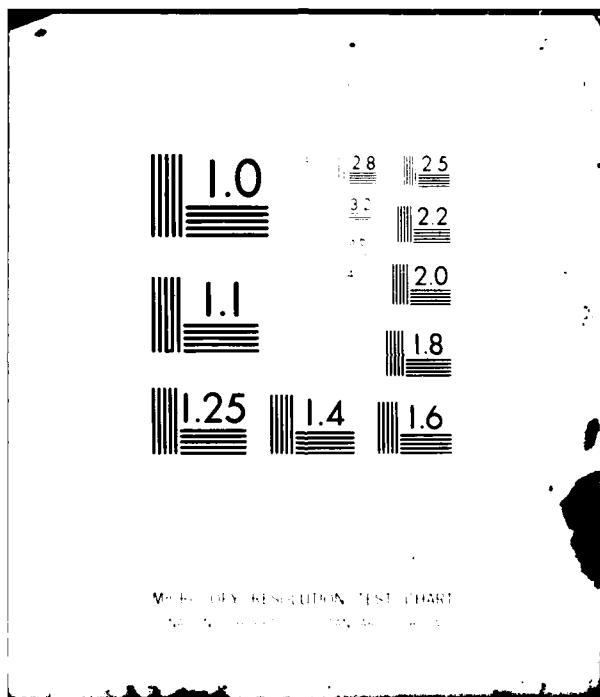
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RANDOM SEQUENTIAL PACKING IN EUCLIDEAN SPACES OF DIMENSIONS
THREE AND FOUR AND A CONJECTURE OF PALASTI

By

B. EDWIN BLAISDELL AND HERBERT SOLOMON

TECHNICAL REPORT NO. 304

JULY 27, 1981



Prepared Under Contract
N00014-76-C-0475 (NR-042-267)
For the Office of Naval Research

Herbert Solomon, Project Director

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| NTIS GRAAT | <input checked="" type="checkbox"/> |
| DTIC File No. | |
| Universal Leader | <input type="checkbox"/> |
| Journal Reference | |
| Report Date | |
| Author(s) | |
| Editor(s) | |
| Avail. by Report/ | |
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RANDOM SEQUENTIAL PACKING IN EUCLIDEAN SPACES
OF DIMENSIONS THREE AND FOUR
AND A CONJECTURE OF PALASTI

By

B. Edwin Blaisdell and Herbert Solomon

INTRODUCTION.

Random sequential packing of hypercubes in a larger hypercube and a conjecture of Palasti [11] that the limiting density β_d in a space of dimension d equals β^d where β is the limiting packing density in one dimension, i.e., on a line, continues to be studied, but with inconsistent results. Rényi [12] and Dvoretzky and Robbins [5] have derived an integral-difference equation for β and Blaisdell and Solomon [3], in an investigation of the Palasti conjecture, have calculated the value of β to 14 significant digits, for purposes of this paper approximately 0.7476. In that paper, we have also studied packing on finite lattices with rigid boundaries by computer experiment in one and two dimensions. In one dimension our results were in good agreement with our extension of an analytic result of Mackenzie [10] for lattice lines, namely

$$(1) \quad c = 1 - [1 + a/n + O(2^{n/2}/(n/a)!)] [k_0 - k_1 a^{-1} + O(a^{-2})]$$

where $\beta = \lim c$ as $a n^{-1} \rightarrow 0$ and $a^{-1} \rightarrow 0$,

and $k_0 = 1 - \beta$, $k_1 = \frac{1}{2}[\beta - \exp(-2\gamma)] \approx 0.2162$ and γ is Euler's constant, n is the number of lattice nodes on the bounding lattice line and a is the number of lattice nodes on the edge of the randomly deposited lattice segment. Define

$$(2) \quad x_1 = (1-c)/(1+a/n) - 0.2524 + 0.2162a^{-1}$$

by a partial rearrangement of (1). This permits satisfactory extrapolation of our finite one-dimensional lattice data to the infinite continuum. A least squares treatment of our one-dimensional data in [3] yielded

$$(3) \quad x_1 \approx 0.0000(+0.0001) + 0.0038(\pm 0.0036)a^{-2}$$

where the values in parenthesis are the estimated standard deviations of the preceding estimated parameters. Note that the estimated intercept is zero, thus agreeing with equation (1) (that is, the lattice lines situation). A similar treatment in [3] of our two-dimensional data yielded

$$(4) \quad x_2 = x_d \approx -0.0025(\pm 0.0001) + 0.0109(\pm 0.0023)a^{-2}$$

where x_d is the same as x_1 in equation (2) except that c is replaced by $(c_d)^{1/d}$. The subscript of x indicates the dimensionality of the lattice space. This result is evidence for a small but significant discrepancy when Palasti's conjecture is viewed in two dimensions, i.e., the packing density is larger in two dimensions than Palasti's assertion.

In 1975 Akeda and Hori published a note [1] in which verification of Palasti's conjecture in the plane was asserted on the basis of computer experiments in two dimensions on squares with $n/a = 100$ and

a = the value of the floating point mantissa of their computer, i.e., the "continuous" model. After being informed by us of our paper [3] they carried out further experiments [2], performed the necessary extrapolation to $a/n \rightarrow 0$ and obtained a value $x_2 = -0.0027(+0.0002)$. Akeda and Hori also studied the three-dimensional "continuous" model by a different and undescribed method for values of $a/n = 8, 10, 12, 15, 20$ and 30 and on extrapolation to $a/n \rightarrow 0$ obtained a value $x_3 = 0.0018(+0.0008)$. The discrepancy, x_3 , has a sign opposite to that for two dimensions and the line through the individual points crosses the expected extrapolation line, both results unappealing intuitively.

In 1978 Weiner published a purported proof of the Palasti conjecture [17] but the validity of his proof has been challenged by several correspondents [7,8,13,14,15,16] and we agree that his claim is not valid. Finegold and Donnell [6] published a note in 1979 on computer experiments on the two-dimensional "continuous" model with periodic boundaries by a "fine mesh" and a "coarse mesh" method and asserted verification of the Palasti conjecture. Their three summary values are $x_2 = -0.0027(+0.0005)$, $-0.0040(+0.0005)$ and $-0.0034(+0.0012)$. They assert that the use of periodic boundaries makes it unnecessary to extrapolate to $a/n \rightarrow 0$, a statement which is only true in one-dimension for $\frac{n}{a} > 14$. The accuracy of the approximation is unknown for higher dimensions. In 1980 Jodrey and Tory [9] published the results of extensive computer experiments on the "continuous" model with periodic boundaries for dimensions 1, 2, and 3 and a few results for dimension 4. Their extrapolated values are $x_1 = 0.0004(+0.0005)$, $x_2 = -0.0021(+0.0002)$, and $x_3 = -0.0029(+0.0002)$ and the average of their 3 values for $x_4 = -0.0003(+0.0006)$.

The values of x_2 obtained by three of the sets of authors [2,3,9] are in good agreement -0.0027, -0.0025, and -0.0021 respectively and show a small departure from the Palasti conjecture. The values of x_3 obtained by two of the authors [2,9] are in poor agreement and of opposite sign +0.0018 and -0.0029 respectively.

Several of these authors have also reported the variance of the limiting density and a similar account may be given. In one dimension our results were in good agreement with an analytic result of Mackenzie [5] for the lattice line. Define

$$(5) \quad y_1 = s^2 / [(a/n)(1+a/n)] \rightarrow A_2(a)$$

as $a/n \rightarrow 0$ and $1/a \rightarrow 0$ and $A_2(a)$ is an undetermined power series in $1/a$. A least squares treatment of our one-dimensional data in [3] yielded

$$(6) \quad y_1 = 0.0381(+0.0003) + 0.0161(+0.0065)(1/a) - 0.0422(+0.0238)(1/a)^2$$

where 0.0381 is in good agreement with the result (0.038156) we obtained in [3] by numerical integration of the analytic expression for the continuous line obtained by Dvoretzky and Robbins [5]. A plausible generalization to d dimensions of equation (5), namely

$$(7) \quad y_d = s_d^2 / [(a/n)(1+a/n)]^d$$

TABLE I

Average normalized variances for sequential random packing densities.

| Ref | Dimension | y_d | notes |
|-----------|-----------|---------------------|-------|
| (1) | 2 | 0.0402 ± 0.0213 | a |
| (2) | 2 | 0.0482 ± 0.0135 | a |
| | 3 | 0.0413 ± 0.0206 | |
| | 1 | 0.0400 ± 0.0058 | |
| (9) | 2 | 0.0468 ± 0.0069 | |
| | 3 | 0.0451 ± 0.0101 | |
| | 4 | 0.0324 ± 0.0176 | |
| (3) | 1 | 0.0393 ± 0.0014 | c |
| | 2 | 0.0526 ± 0.0027 | c |
| this work | 3 | 0.0519 ± 0.0062 | |
| | 4 | 0.0518 ± 0.0158 | |

Notes: (a) only the values for squares of edge ≥ 40 have been used.(c) only a subset of the values obtained in (3) have been used,
as described below.

was found by least squares to be in good agreement with our two-dimensional data [3], namely

$$(8) \quad y_2 = 0.0508(\pm 0.0010) + 1.3697(\pm 0.3905)(1/a)^3 - 3.6660(\pm 1.1400)(1/a)^4.$$

Average values for y_d are given in Table I. The factor $1+a/n$ which normalizes for finite hypercube size is not used for experiments with periodic boundaries.

New Developments

We have now conducted experiments in three and four dimensions. In doing so, we have adhered to our earlier policy of studying finite lattices with rigid boundaries. Although this policy results in loss of accuracy when extrapolating to the infinite continuum [9], it is easier to program and permits an exact accounting of every lattice site as occupied or unoccupiable. Authors who have studied the "continuous" case, i.e., have used floating point arithmetic, have not agreed with each other nor with our present results in dimension three. One possible explanation for this is the occurrence of holes that present a very tight fit in at least one dimension, and which have been missed because of round-off error in the continuous case. The likelihood of these tight fits occurring will increase with increasing dimension and may account for Jodrey and Tory [9] finding densities increasingly lower than ours in dimensions two, three and four.

Our calculations were made as described before in [3] except that we now used a DEC PDP11/55 computer running FORTRAN programs under

operating system RSX11M. Lattice points were identified with bits in the computer's 16-bit words, which permitted use of hypercubes containing up to 70^3 or 24^4 (about 330,000) lattice nodes. The new values obtained in dimensions three and four are given in Table II. These values together with subsets of those obtained formerly in [3] in dimensions one and two have been treated together since a regular pattern related to dimension has become apparent. For dimension one we used values for $a \leq 100$, $n/a \leq 20$ and for dimension two, values for $a \leq 20$, $n/a \leq 10$. This yielded sets of about the same number for each of the four dimensions so that the large number of values otherwise available for dimensions one and two would not outweigh those calculated for dimensions three and four. The numbers for dimensions one, two, three, and four are respectively 28, 34, 51, and 32 including all values, and 18, 22, 30, and 24 excluding values for $a = 2$ and $n/a = 5$ which we found as before [3] to require more terms in the expansion of equation (1) for obtaining a satisfactory fit.

We have examined our results guided by the theoretical equation (2) for one dimension, substituting for c , the value $c_d^{1/d}$, (the Palasti conjecture) in higher dimensions. The results of our examination are given in Table III. Lines 1, 2, 3, and 4 contain the least squares results treating each dimension separately. It is apparent that the intercept (a measure of the departure from the Palasti conjecture) increases rather regularly with dimension and that the coefficient of the term in $1/a^2$ (a measure of the departure from the limiting equation (2)) decreases with dimension. Lines 5, 6, 7, and 8 contain

TABLE II

| n/a | Lattice Dimension 3 | | | | | | Lattice Dimension 4 | | | | | | |
|-----|---------------------|-----------------|-------------|-----------------|-------------|-----------------|---------------------|-------------|-----------------|-------------|-----------------|-------------|-----|
| | $10^4 \rho$ | $10^4 \sigma^2$ | $10^4 \rho$ | $10^4 \sigma^2$ | $10^4 \rho$ | $10^4 \sigma^2$ | n/a | $10^4 \rho$ | $10^4 \sigma^2$ | $10^4 \rho$ | $10^4 \sigma^2$ | $10^4 \rho$ | |
| 14 | | | 3763 | 2860 | | | 4 | | | 3696 | 109 | 3576 | 384 |
| 13 | | | 3806 | 2394 | | | 4 | | | 3676 | 213 | 3588 | 377 |
| 12 | | | 3838 | 2766 | | | 4 | | | 3686 | 119 | | |
| 11 | | | 3961 | 1241 | 3858 | 2800 | 4 | | | 3692 | 210 | | |
| 11 | | | 3956 | 1513 | | | 4 | | | 3706 | 203 | | |
| 11 | | | 3961 | 1610 | | | 4 | | | 3680 | 209 | | |
| 11 | | | 3955 | 1427 | | | 4 | | | 3694 | 108 | | |
| 10 | 4104 | 724 | 3999 | 1458 | 3924 | 2728 | 4 | | | 3709 | 237 | | |
| 10 | 4092 | 902 | | | | | 4 | | | 3680 | 223 | | |
| 10 | 4109 | 733 | | | | | 4 | | | 3662 | 298 | | |
| 10 | 4072 | 918 | | | | | 4 | | | 3694 | 161 | | |
| 10 | 4108 | 777 | | | | | 4 | | | 3693 | 130 | | |
| 9 | 4136 | 816 | 4046 | 1447 | 3947 | 2740 | 3 | 4212 | 105 | 4128 | 130 | 4040 | 308 |
| 8 | 4201 | 589 | 4139 | 1224 | 3988 | 2730 | 3 | 4185 | 112 | 4115 | 161 | 4022 | 380 |
| 7 | 4257 | 686 | 4197 | 1268 | 4076 | 1785 | 3 | 4207 | 54 | 4154 | 228 | | |
| 6 | 4385 | 776 | 4296 | 1400 | 4196 | 2498 | 3 | 4180 | 64 | 4102 | 216 | | |
| 5 | 4531 | 745 | 4435 | 1322 | 4346 | 2115 | 3 | 4196 | 94 | | | | |
| 5 | 4520 | 906 | 4442 | 1410 | 4342 | 2345 | 3 | 4203 | 78 | | | | |
| 4 | 4765 | 704 | 4692 | 1144 | 4591 | 2517 | 3 | 4216 | 84 | | | | |
| 4 | 4767 | 603 | 4683 | 1116 | 4576 | 2336 | 3 | 4193 | 151 | | | | |
| 3 | 5160 | 619 | 5109 | 944 | 4993 | 2119 | 2 | | | 5153 | 198 | 5064 | 388 |
| 3 | 5182 | 719 | 5102 | 1221 | 5005 | 1739 | 2 | | | 5136 | 121 | 5077 | 365 |
| 2 | 6089 | 608 | 6062 | 861 | 5954 | 1813 | | | | | | | |
| 2 | 6089 | 454 | 6049 | 709 | 5963 | 2079 | | | | | | | |

TABLE III

Least squares expressions for $10^4 x_d$, $x_d = 0.2524 - (0.2162/a) - (1-c_d^{1/d})/(1+a/n)$

| expression | # ^{ref} | dim | data excluded | #data points | resid sum squares | std error of estimate | F | C_p | Mallow's * |
|--|------------------|-----------|---------------|--------------|-------------------|-----------------------|------|-------|------------|
| 1 $-1.6 \pm 1.5 + 4.71 \pm 50(1/a^2)$ | 1 | a=2,n/a=5 | 18 | 433 | 5.05 | 126 | | | |
| 2 $24.7 \pm 2.2 + 304 \pm 42(1/a^2)$ | 2 | a=2,n/a=5 | 22 | 943 | 6.86 | 331 | | | |
| 3 $51.5 \pm 1.5 + 257 \pm 30(1/a^2)$ | 3 | a=2,n/a=5 | 30 | 904 | 5.68 | 1764 | | | |
| 4 $85.7 \pm 4.9 + 110 \pm 54(1/a^2)$ | 4 | a=2,n/a=5 | 24 | 918 | 6.46 | 2612 | | | |
| 5 0 $(d-1) + 437 \pm 34(1/(a^2\sqrt{d}))$ | 1 | a=2,n/a=5 | 18 | 433 | 5.05 | 126 | | | |
| 6 $24.73 \pm 2.16(d-1) + 430 \pm 60(1/(a^2\sqrt{d}))$ | 2 | a=2,n/a=5 | 22 | 943 | 6.86 | 331 | | | |
| 7 $25.77 \pm 0.76(d-1) + 446 \pm 53(1/(a^2\sqrt{d}))$ | 3 | a=2,n/a=5 | 30 | 904 | 5.68 | 1764 | | | |
| 8 $28.58 \pm 1.63(d-1) + 219 \pm 108(1/(a^2\sqrt{d}))$ | 4 | a=2,n/a=5 | 24 | 918 | 6.46 | 2612 | | | |
| 9 $25.84 \pm 0.49(d-1) + 414 \pm 27(1/(a^2\sqrt{d}))$ | all 1 | a=2,n/a=5 | 94 | 3376 | 6.06 | 4986 | 5.75 | | |
| 10 $26.55 \pm 0.42(d-1) + 385 \pm 12(1/(a^2\sqrt{d}))$ | all 1 | n/a=5 | 106 | 5178 | 7.06 | 5083 | 19.9 | | |
| 11 $26.68 \pm 0.47(d-1) + 409 \pm 26(1/(a^2\sqrt{d}))$ | all 1 | a=2 | 127 | 5733 | 6.77 | 5373 | 24.8 | | |
| 12 $27.15 \pm 0.39(d-1) + 399 \pm 10(1/(a^2\sqrt{d}))$ | all 1 | none | 145 | 8083 | 7.52 | 6410 | 50.3 | | |
| 13 $25.49 \pm 1.13(d-1) + 392 \pm 68(1/(a^2\sqrt{d})) + 112 \pm 325(a/n)(1/a^2) + 3 \pm 12(a/n)$ | all 1 | a=2,n/a=5 | 94 | 3370 | 6.12 | 2443 | 7.69 | | |
| 14 $24.54 \pm 0.91(d-1) + 299 \pm 24(1/(a^2\sqrt{d})) + 538 \pm 130(a/n)(1/a^2) + 12 \pm 12(a/n)$ | all 1 | n/a=5 | 106 | 4429 | 6.59 | 2918 | 6.27 | | |
| 15 $24.03 \pm 0.76(d-1) + 276 \pm 56(1/(a^2\sqrt{d})) + 493 \pm 237(a/n)(1/a^2) + 33.6 \pm 7.8(a/n)$ | all 1 | a=2 | 127 | 4943 | 6.34 | 3071 | 8.46 | | |
| 16 $23.85 \pm 0.64(d-1) + 289 \pm 26(1/(a^2\sqrt{d})) + 520 \pm 91(a/n)(1/a^2) + 32.4 \pm 7.5(a/n)$ | all 1 | none | 145 | 6070 | 6.56 | 4220 | 6.69 | | |

* see Ref 4

the least squares results treating each dimension separately but including least squares estimates of these observed trends. The fit is of course the same but the near constancy of the respective parameter estimates shows that the model form is satisfactory.

Lines 9, 10, 11, and 12 contain least squares results treating all dimensions at once but successively adding the less well fitted values for $a = 2$ and $n/a = 5$. The standard error of estimate increases about 25% but the F value increases about 30%, because of the substantial increase in degrees of freedom, as these values are included. A search was made for further terms which might significantly improve the fit using program P9R, all possible subsets regression, of the BMDP package [4]. Lines 13, 14, 15, and 16 contain the least squares results for the best choice of 4 terms from the following: $(d-1)$, $1/a$, a/n , $1/a^2$, $1/a^3$, $1/a^4$, $1/(a^2\sqrt{d})$, $(a/n)(1/a^2)$. The additional terms make a significant improvement in the standard error of estimate if the data for $a = 2$ or $n/a = 5$ are included but not otherwise.

The residuals from the fit in line 9 are plotted against $(d-1)$ in Figure 1 and against $1/(a^2\sqrt{d})$ in Figure 2. The plotted digits show the number of superposed values at that location. There appears to be no trend in the residuals with either term, further testimony that the model is satisfactory.

Computer experiments on the random sequential packing of finite lattices with rigid boundaries in dimensions one, two, three and four indicate a discrepancy with the Palasti conjecture in the limit $1/a \rightarrow 0$, $a/n \rightarrow 0$ which increases about 0.0025 in $c_d^{1/d}$ per dimension. These

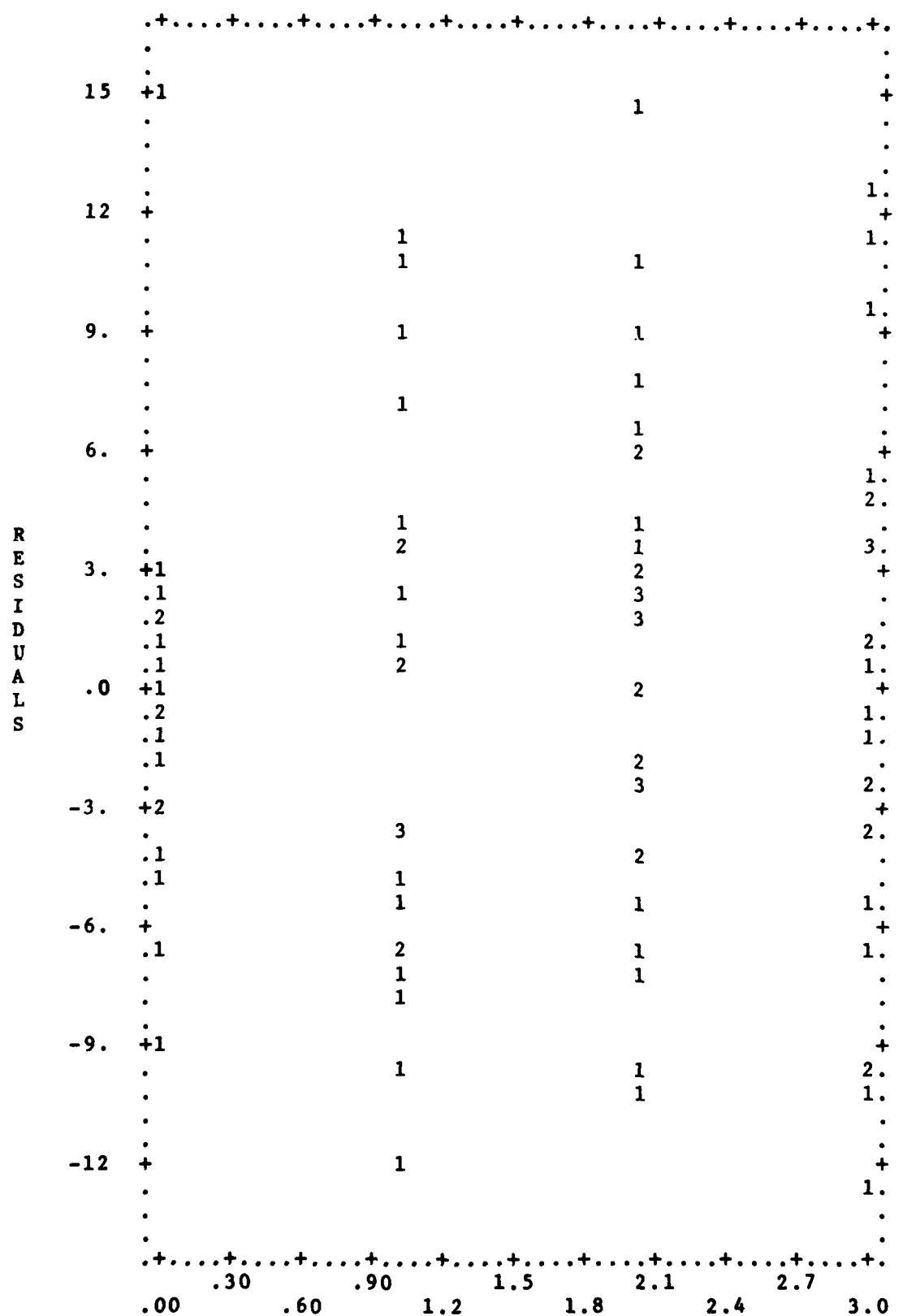
correspond to discrepancies for dimensions two, three and four of 0.0037, 0.0084, and 0.0127 in the density itself, c_d being greater than c_1^d . This may be seen by a rearrangement of the limiting form of equation (2) with c replaced by $c_d^{1/d}$. We can now write $c_d^{1/d} - c_1 = z(d-1)$ where the right side is the limiting expression found in Table III. Then

$$c_d = [c_1 + z(d-1)]^d$$

or

$$c_d - c_1^d = z c_1^{d-1} d(d-1) + \frac{z^2}{2} c_1^{d-2} d(d-1)^3 + \frac{z^3}{6} c_1^{d-3} d(d-1)^4 (d-2) + \dots$$

where $c_1 \approx .7476$ and $z = \sqrt{c_2} - c_1 \approx .0025$, the excess over the value given by the Palasti conjecture when $d = 2$. Note that the expansion truncates at $(d+1)$ terms and because $z \approx .0025$ is quite small, no terms beyond the first are significant to four decimal places and this leads to the discrepancies for dimensions two, three, and four given above.



(d-1)
Figure 1

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| 4. TITLE (and Subtitle) RANDOM SEQUENTIAL PACKING IN EUCLIDEAN SPACES OF DIMENSIONS THREE AND FOUR AND A CONJECTURE OF PALASTI | 5. TYPE OF REPORT & PERIOD COVERED TECHNICAL REPORT | |
| 7. AUTHOR(s) B. EDWIN BLAISDELL AND HERBERT SOLOMON | 6. PERFORMING ORG. REPORT NUMBER N00014-76-C-0475 | |
| 9. PERFORMING ORGANIZATION NAME AND ADDRESS Department of Statistics Stanford University Stanford, CA 94305 | 10. PROGRAM ELEMENT, PROJECT, TASK AREA & WORK UNIT NUMBERS NR-042-267 | |
| 11. CONTROLLING OFFICE NAME AND ADDRESS Office Of Naval Research Statistics & Probability Program Code 436 Arlington, VA 22217 | 12. REPORT DATE JULY 27, 1981 | 13. NUMBER OF PAGES 15 |
| 14. MONITORING AGENCY NAME & ADDRESS (if different from Controlling Office) | 15. SECURITY CLASS. (of this report) UNCLASSIFIED | |
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RANDOM SEQUENTIAL PACKING IN EUCLIDEAN SPACES OF DIMENSIONS THREE AND FOUR AND A CONJECTURE OF PALASTI

A conjecture of Palasti [11] that the limiting packing density β_d is a space of dimension d equals β^d where β is the limiting packing density in one dimension continues to be studied, but with inconsistent results. Some recent correspondence to this Journal [7,8,13,14,15,16,18,19,20] as well as some other papers indicate a lively interest in the subject. In a prior study [3], we demonstrated that the conjectured value in two dimensions was smaller than the actual density. Here we demonstrate that this is also so in three and four dimensions and that the discrepancy increases with dimension.

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